A comparative study of two-phase equilibria modeling tools: MORB equilibrium states at variable pressure and H₂O concentrations

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ABSTRACT

Phase equilibria modeling is a powerful petrological tool to address both forward and inverse geological problems over a broad range of crustal and upper mantle conditions of pressure (P), temperature (T), composition (X), and redox (f_{O_2}). The development of thermodynamic databases, relatively realistic activity−composition ($a−X$) relations for solids, melts and fluids, pressure-volume-temperature (PVT) equations of state (EOS), and efficient numerical algorithms represent an inflection point in our ability to understand the nexus between tectonics and petrogenesis. While developed—and typically applied in isolation—by either metamorphic or igneous petrologists, some of the published thermodynamic models have overlapping P-T-X calibration ranges, which enables comparisons of model outcomes for similar conditions within the range of applicability. In this paper, we systematically compare the results of two such models that are routinely used for calculating phase equilibria in melt-bearing systems: rhyolite-MELTS (Gualda et al. 2012; Ghiorso and Gualda 2015) and the metabasite set of Green et al. (2016) using the thermodynamic database ds62 (Holland and Powell 2011) (hereafter denoted as "HPx-mb16"). We selected a N-MORB composition and modeled closed system equilibrium phase relations as a function of temperature at 0.25 and 1 GPa for N-MORB with 0.5 and 4 wt% H₂O. Our results show that phase relations exhibit some key differences that, in some instances, impact geological inferences. For example, clinopyroxene and plagioclase stabilities are expanded to higher temperatures in HPx-mb16 compared to predictions from rhyolite-MELTS. Orthopyroxene and olivine are stable in greater proportions and at wider temperature ranges in rhyolite-MELTS compared to HPx-mb16. Importantly, HPx-mb16 predicts amphibole in all runs presented here, whereas amphibole is only predicted at high-P–high-H₂O (1 GPa and 4 wt% H₂O) in rhyolite-MELTS, and in lesser amounts. Garnet stability is systematically expanded at higher temperatures, and the proportion is greater in rhyolite-MELTS. In addition to phase assemblage differences, phase compositions may differ. For example, plagioclase anorthite content is systematically higher in HPx-mb16 (for the same set of conditions), whereas garnet Mg# is higher in rhyolite-MELTS. Calculated amphibole compositions are substantially different between the two models as well. Liquid compositions also show important differences. High-T liquids are generally similar in SiO₂ contents but diverge at lower temperatures; in these cases, HPx-mb16 liquids are SiO₂-depleted compared to those produced by rhyolite-MELTS. Liquids are also systematically and substantially more mafic in HPx-mb16, and alumina and the alkali concentrations are relatively different and show different trends as a function of temperature at constant pressure. Overall, liquid compositions show the greatest differences near the solidus. Differences in modal abundances of phases and liquid compositions influence liquid trace-element signatures, and these differences can affect geological interpretations. Finally, a comparison between melting experiments of basaltic bulk composition and both thermodynamic models shows that rhyolite-MELTS better reproduces the higher temperature experiments, whereas HPx-mb16 better reproduces the lower temperature experiments. We discuss these and other similarities and differences to highlight the strengths and limitations of each model and to recognize that modeling results have important implications for interpretations of geologic processes. We recognize that our results are informed by a small subset of calculations over a limited range of conditions—but encourage further comparisons over a wider range of conditions and compositions.

Keywords: Phase equilibria modeling, computational petrology, rhyolite-MELTS, Theriak-Domino, thermodynamics